

Supplementary information
for
CuAAC synthesis and structural characterization of
4-carboxymethyl-substituted 1,2,3-triazoles

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Experimental section

Figure 1. ¹H NMR spectrum of 2b (DMSO-d₆, 500 MHz)

Figure 2. ¹³C NMR spectrum of 2b (DMSO-d₆, 125 MHz)

Figure 3. ¹³C-dept ¹³⁵NMR spectrum of 2b (DMSO-d₆, 125 MHz)

Figure 4. ATR-IR spectrum of 2b

Figure 5. MS spectrum of 2b 6

Figure 6. ¹H NMR spectrum of 2c (DMSO-d₆, 500 MHz)

Figure 7. ¹³C NMR spectrum of 2c (DMSO-d₆, 125 MHz)

Figure 8. ¹³C-dept ¹³⁵NMR spectrum of 2c (DMSO-d₆, 125 MHz)

Figure 9. ATR-IR spectrum of 2c

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Figure 11. ¹H NMR spectrum of 2d (DMSO-d₆, 500 MHz)

Figure 12. ¹³C NMR spectrum of 2d (DMSO-d₆, 125 MHz)

Figure 13. ¹³C-dept ¹³⁵NMR spectrum of 2d (DMSO-d₆, 125 MHz)

Figure 14. ATR-IR spectrum of 2d

Figure 15. MS spectrum of 2d

Figure 16. ¹H NMR spectrum of 2e (DMSO-d₆, 500 MHz)

Figure 17. ¹³C NMR spectrum of 2e (DMSO-d₆, 125 MHz)

Figure 18. ¹³C-dept ¹³⁵ NMR spectrum of 2e (DMSO-d₆, 125 MHz)

Figure 19. ATR-IR spectrum of 2e

Figure 20. MS spectrum of 2e

Figure 21. ¹H NMR spectrum of 2f (DMSO-d₆, 500 MHz)

Figure 23. ¹³C-dept ¹³⁵ NMR spectrum of 2f (DMSO-d₆, 125 MHz)

Figure 24. ATR-IR spectrum of 2f

Figure 25. MS spectrum of 2f

Figure 26. ¹H NMR spectrum of 2g (DMSO-d₆, 500 MHz)

Figure 27. ¹³C NMR spectrum of 2g (DMSO-d₆, 125 MHz)

Figure 28. ¹³C-dept ¹³⁵ NMR spectrum of 2g (DMSO-d₆, 125 MHz)

Figure 29. ATR-IR spectrum of 2g

Figure 30. MS spectrum of 2g

Experimental section

Starting materials are commercially available and were used without further purification (suppliers: Carlo Erba Reagents S.A.S., Tokyo Chemical Industry Co. Ltd. and Acros Organics). Melting points were measured on an MPA 100 OptiMelt® apparatus and are uncorrected. Nuclear Magnetic Resonance (NMR) spectra were acquired at 500 MHz for ^1H NMR and at 125 MHz for ^{13}C NMR, on a Bruker Avance III 500 MHz spectrometer (Bruker BioSpin GmbH, Rheinstetten, Germany) with tetramethylsilane (TMS) as internal standard, at 25 °C. Chemical shifts (δ) are expressed in part per million (ppm) relative to the residual solvent signal (2.50 ppm for DMSO- d_6) in ^1H NMR spectra and (39.52 ppm for DMSO- d_6) in ^{13}C NMR spectra, respectively. Splitting patterns are designed as: s, singlet; d, doublet; dd, doublet of doublet; t, triplet; m, multiplet; q, quintuplet; br s, broaden singlet; br t, broaden triplet. Coupling constants (J) are reported in Hertz (Hz). Thin layer chromatography (TLC) was realized on Macherey Nagel silica gel plates with fluorescent indicator and were visualized under a UV-lamp at 254 nm and 365 nm. IR spectra were recorded on a FTIR Bruker Tensor 27 spectrometer. MALDI-TOF MS spectra were acquired on a Bruker Rapiflex MALDI-TOF mass spectrometer equipped with a Smartbeam 3D laser FlexControl (Bruker Daltonics, Version 4.0) operated in positive reflectron ion mode. Samples (20 $\mu\text{g/mL}$ in 0.1% TFA) were mixed 1:1 with a freshly prepared sDHB matrix solution (50 mg/mL in ACN/0.1% TFA in H_2O , 3v : 2v), and 1 μL of the mixture was deposited on a stainless-steel target plate and air dried at room temperature. External calibration was performed using the Bruker Peptide Calibration Standard Kit.

Methyl 1-(2-([1,1'-biphenyl]-4-yl)-2-oxoethyl)-1H-1,2,3-triazole-4-carboxylate (2b)

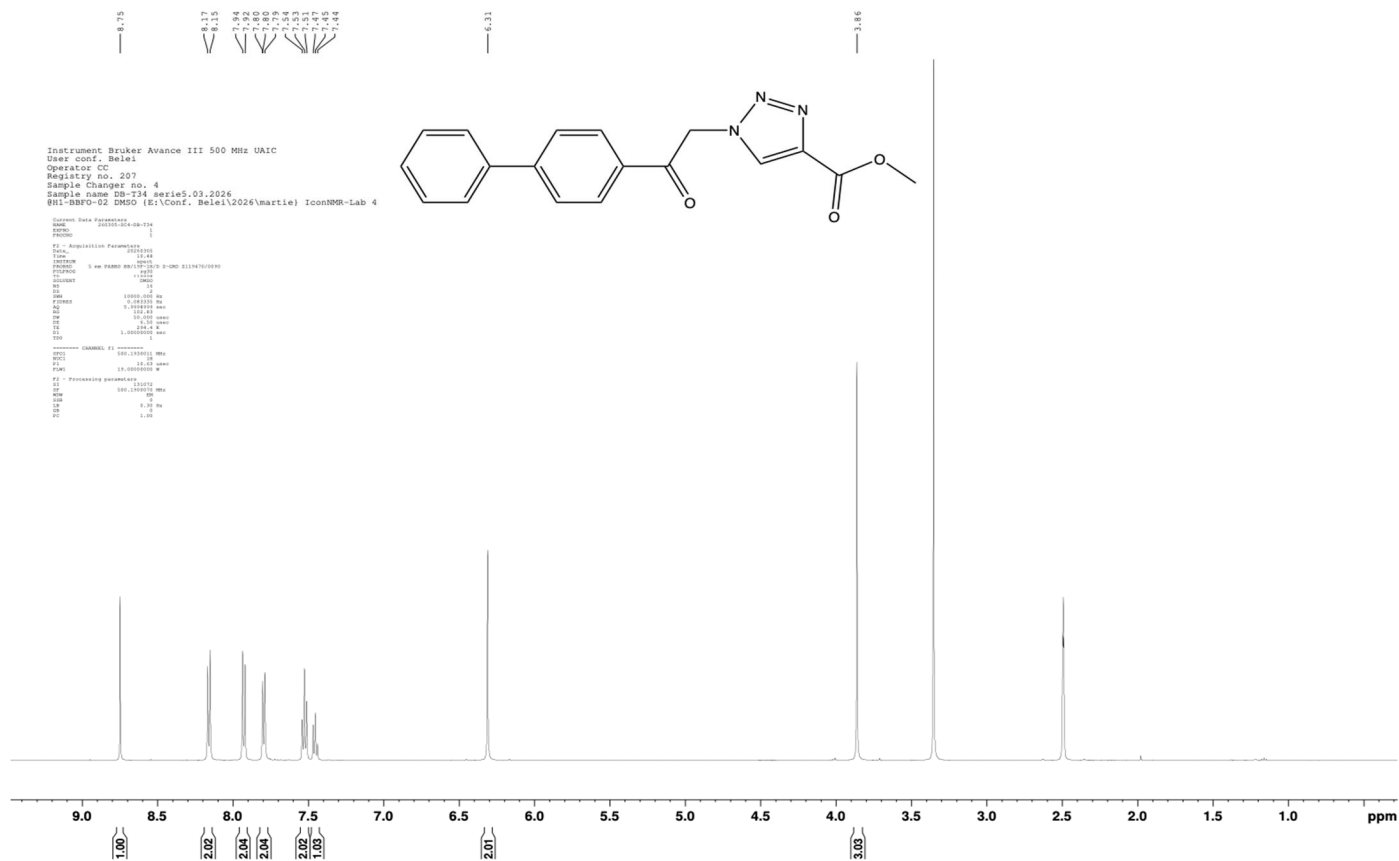


Figure 1. ¹H NMR spectrum of 2b (DMSO-*d*₆, 500 MHz).

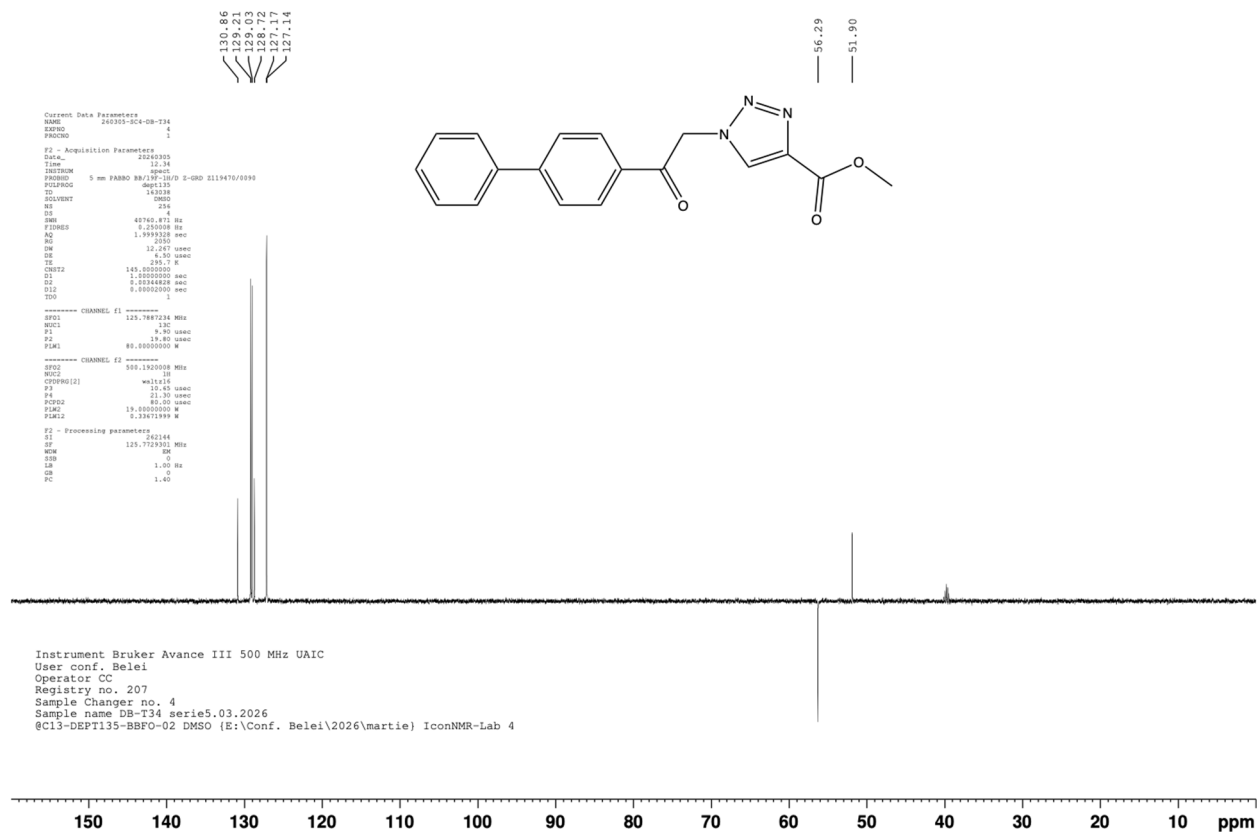


Figure 3. ¹³C-dept 135 NMR spectrum of **2b** (DMSO-*d*₆, 125 MHz).

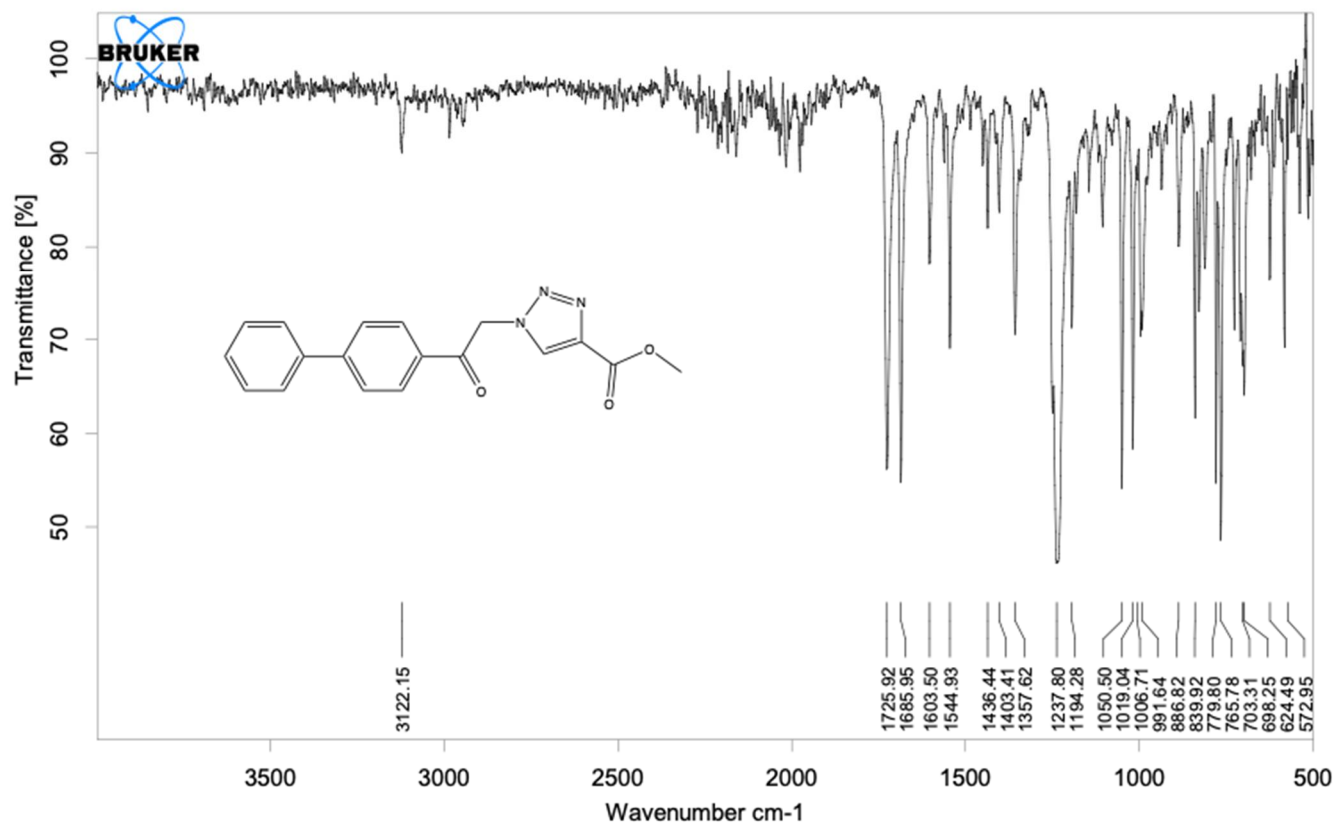


Figure 4. ATR-IR spectrum of **2b**.

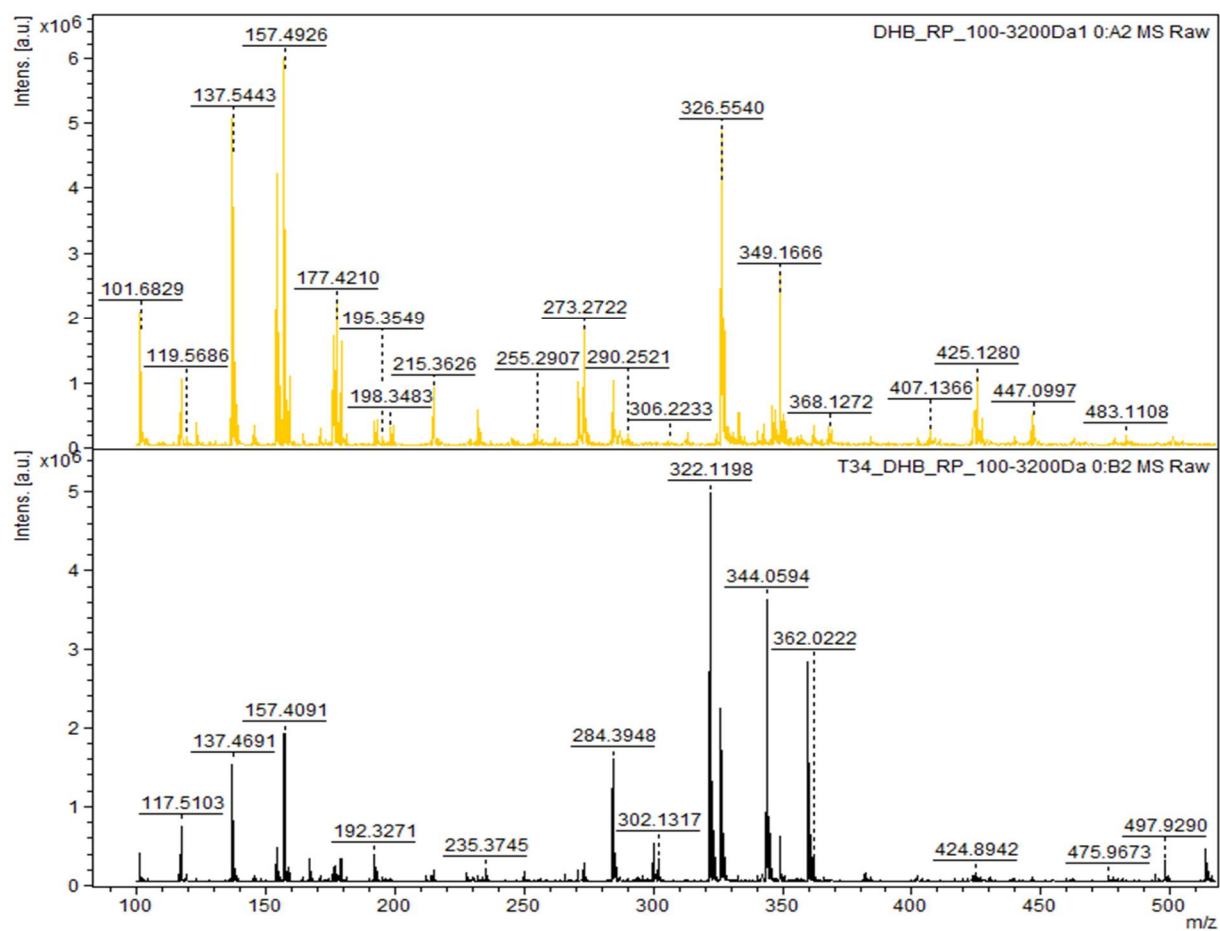


Figure 5. MS spectrum of 2b.

Methyl 1-(2-(4-fluorophenyl)-2-oxoethyl)-1*H*-1,2,3-triazole-4-carboxylate (2c**)**

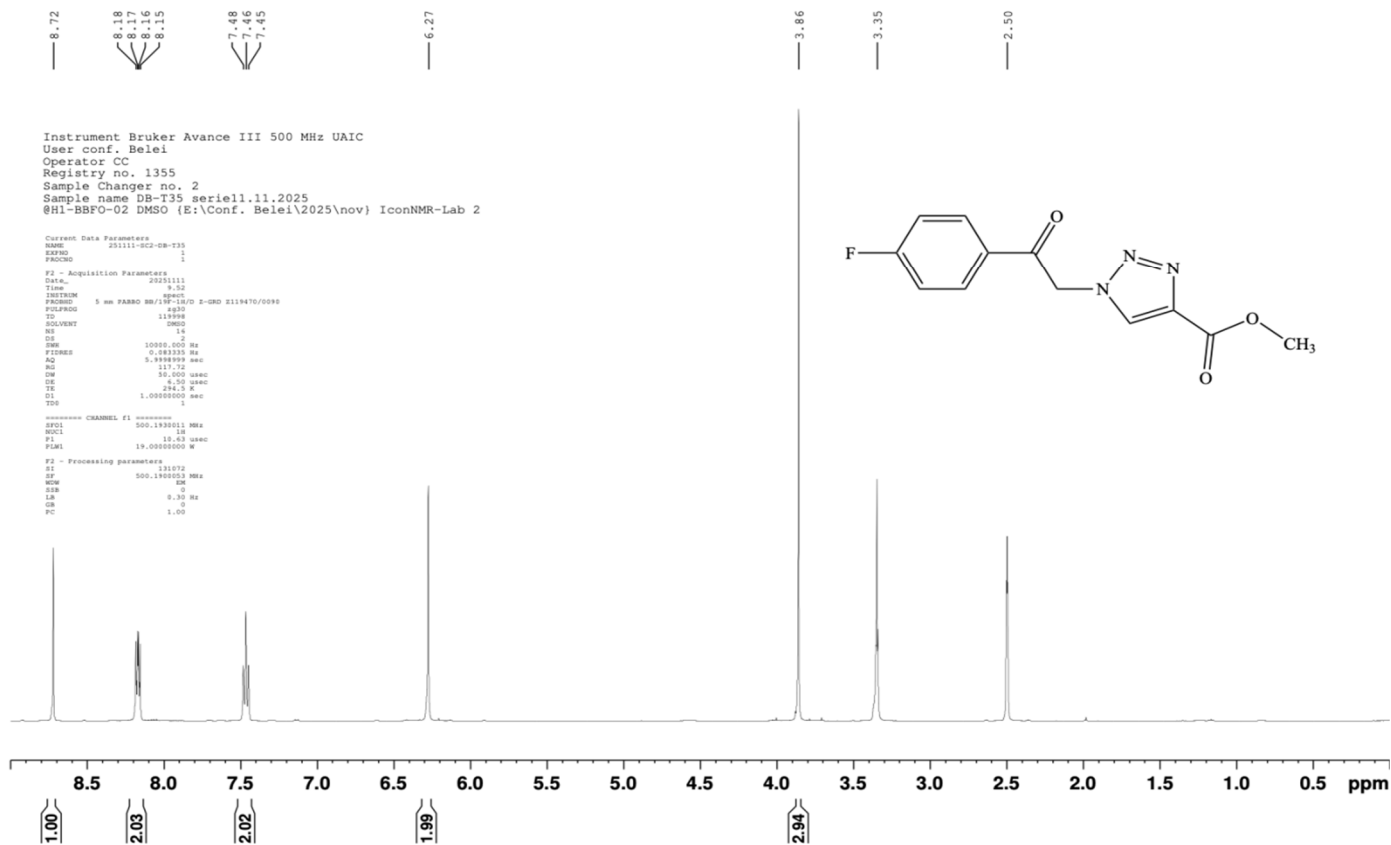


Figure 6. ¹H NMR spectrum of **2c** (DMSO-*d*₆, 500 MHz).



Figure 7. ^{13}C NMR spectrum of 2c (DMSO- d_6 , 125 MHz).

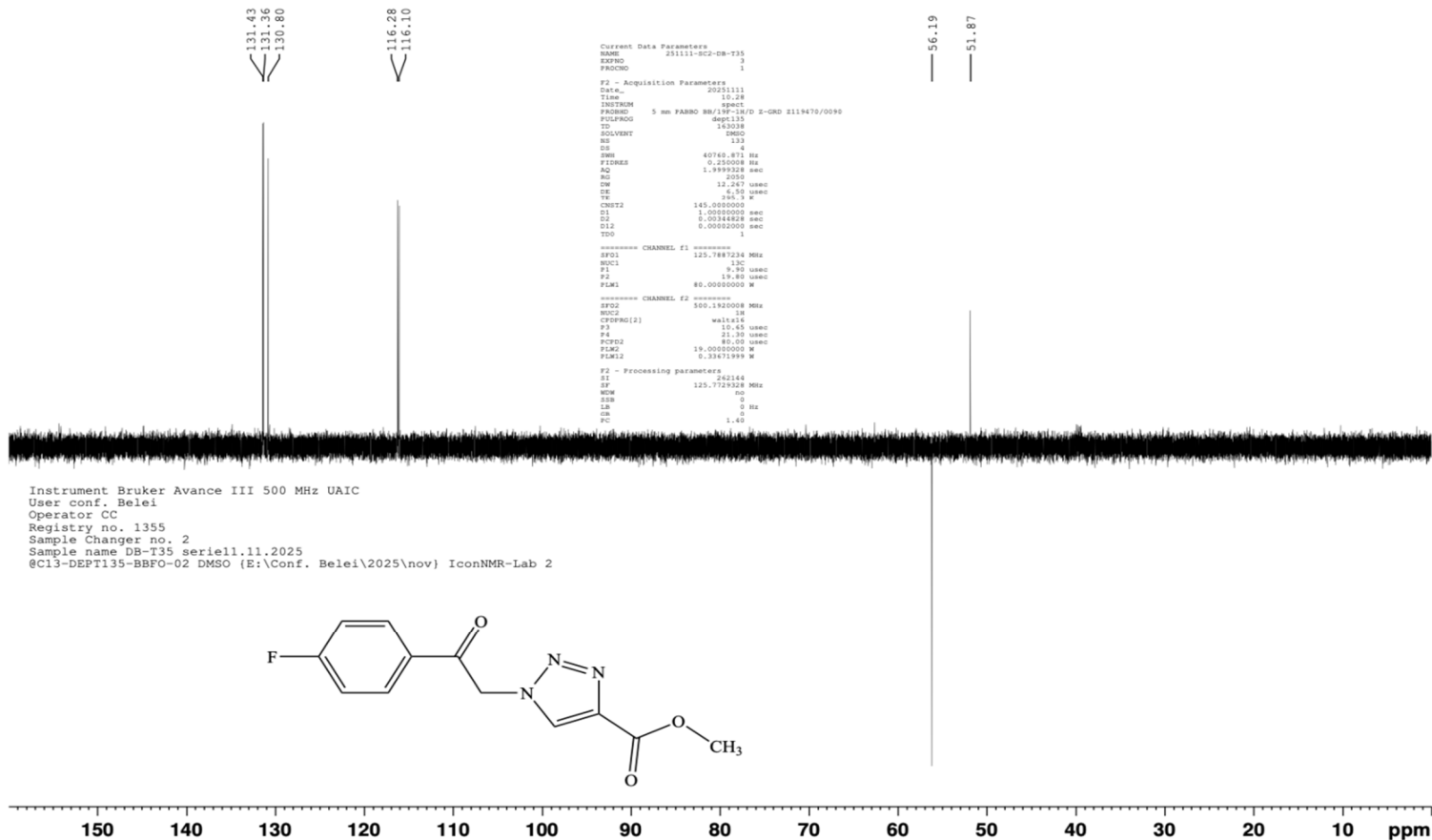


Figure 8. ^{13}C -dept 135 NMR spectrum of **2c** (DMSO- d_6 , 125 MHz).

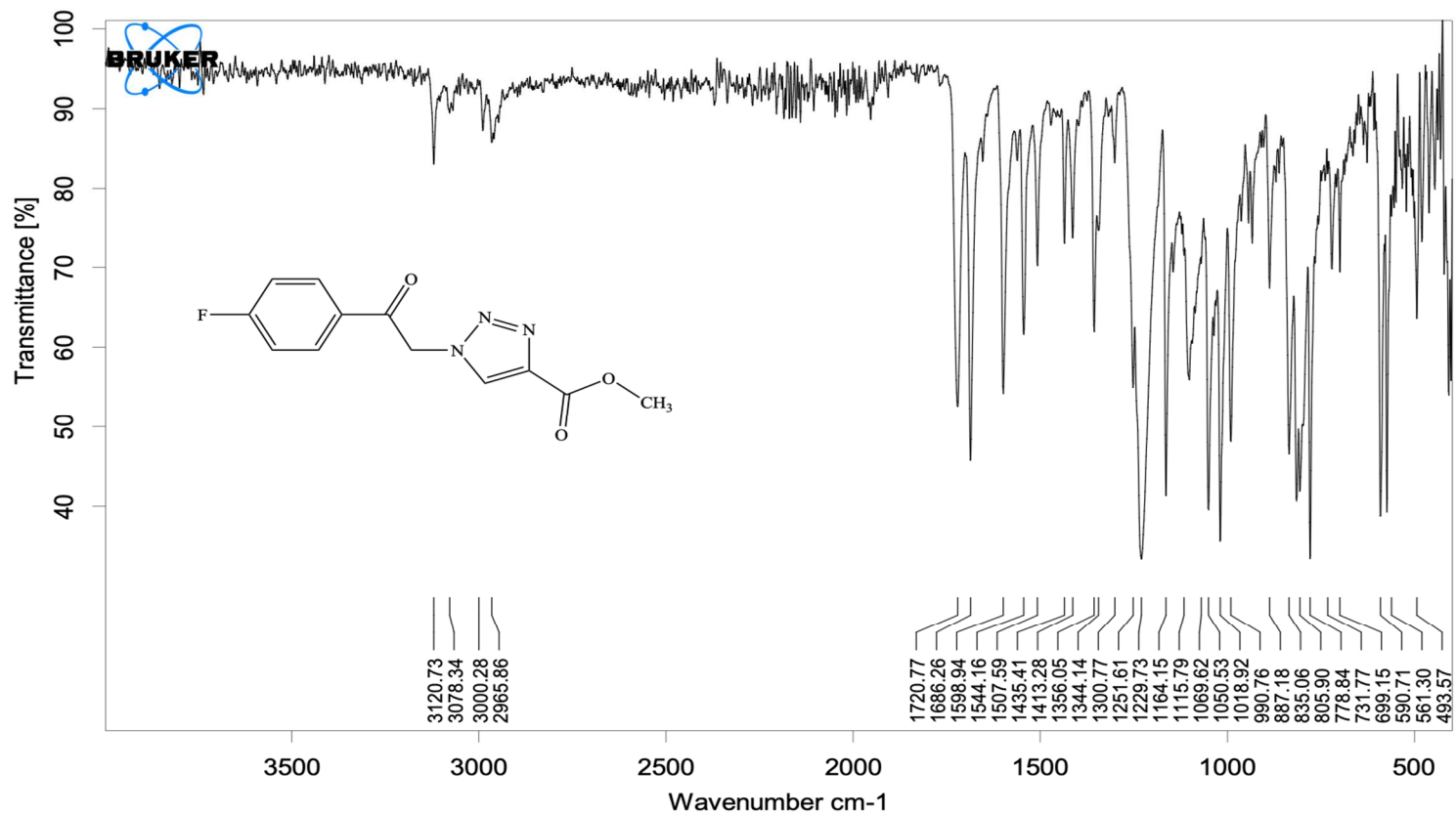


Figure 9. ATR-IR spectrum of 2c.

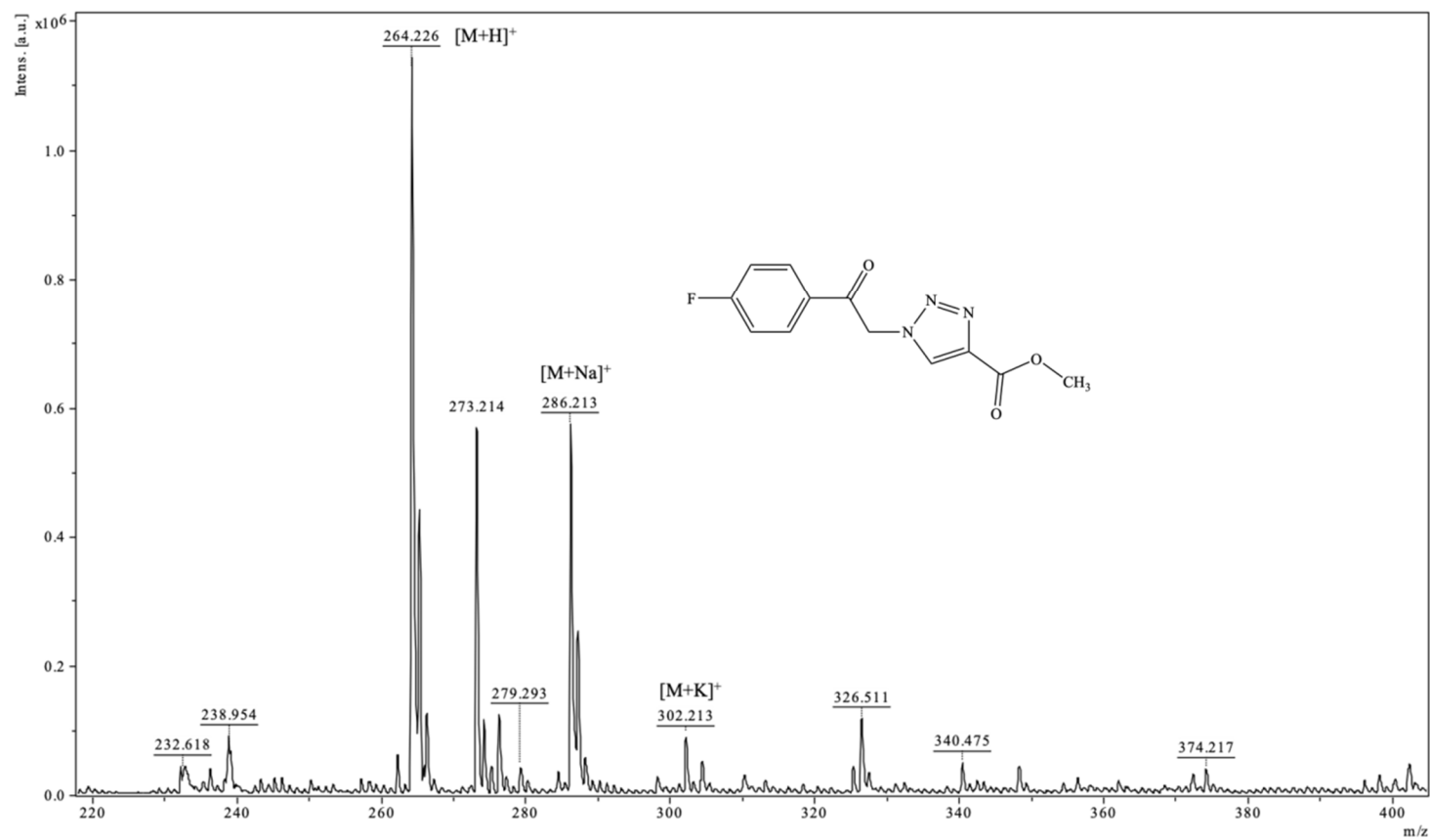


Figure 10. MS spectrum of **2c**.

Methyl 1-(2-oxo-2-(p-tolyl)ethyl)-1H-1,2,3-triazole-4-carboxylate (2d)

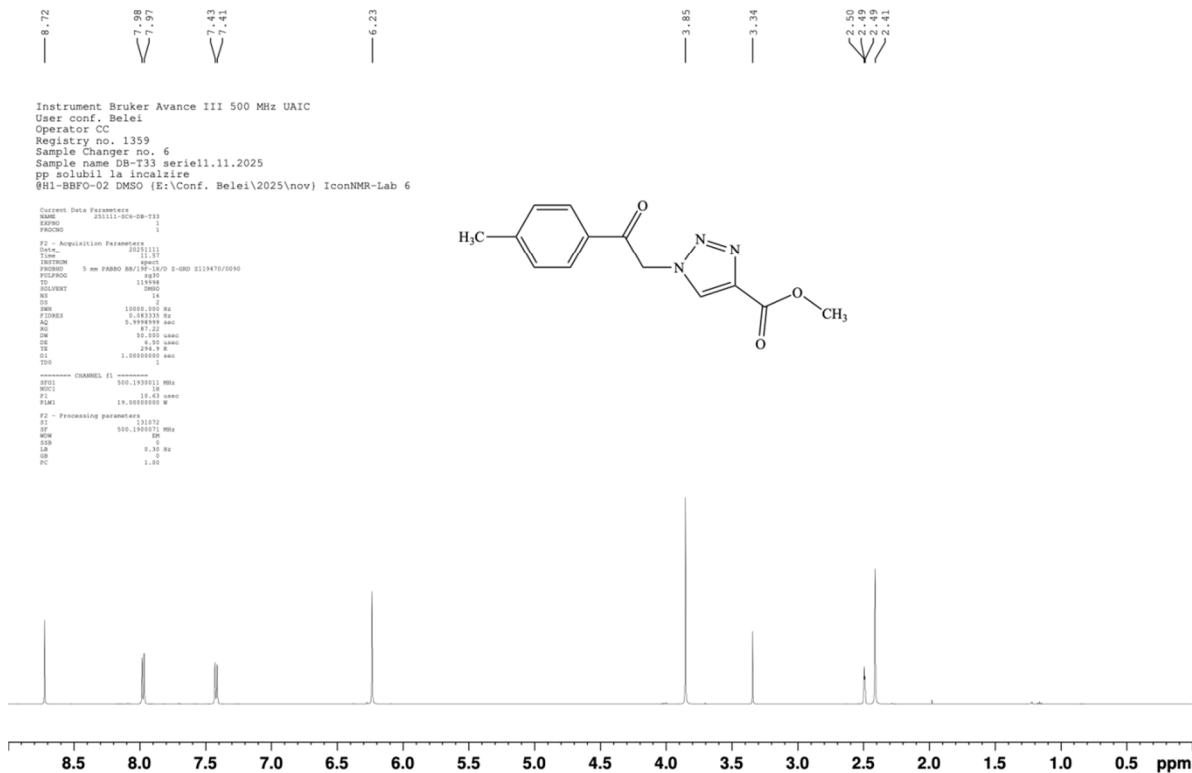


Figure 11. ^1H NMR spectrum of **2d** (DMSO- d_6 , 500 MHz).

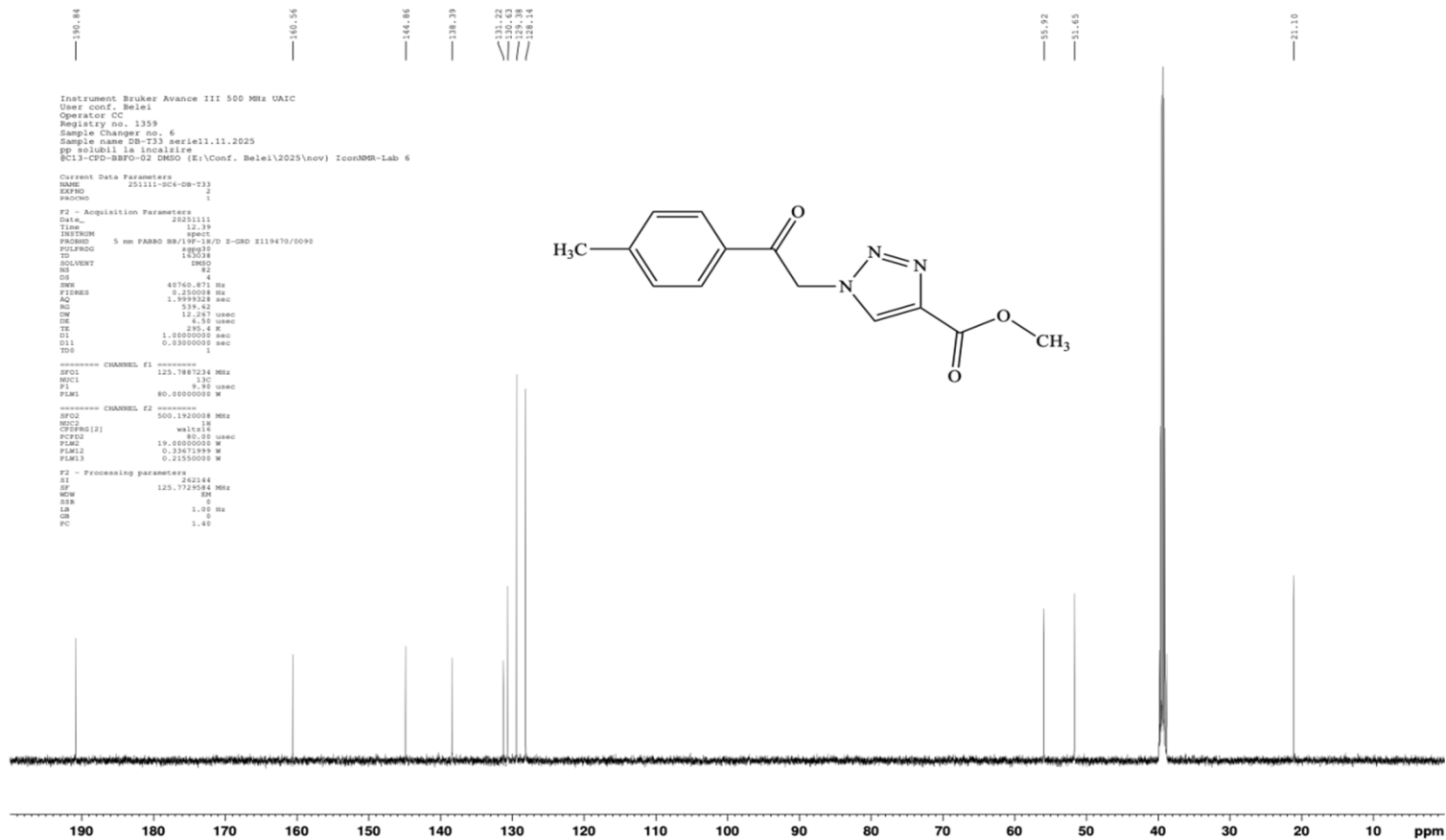


Figure 12. ¹³C NMR spectrum of 2d (DMSO-*d*₆, 125 MHz).

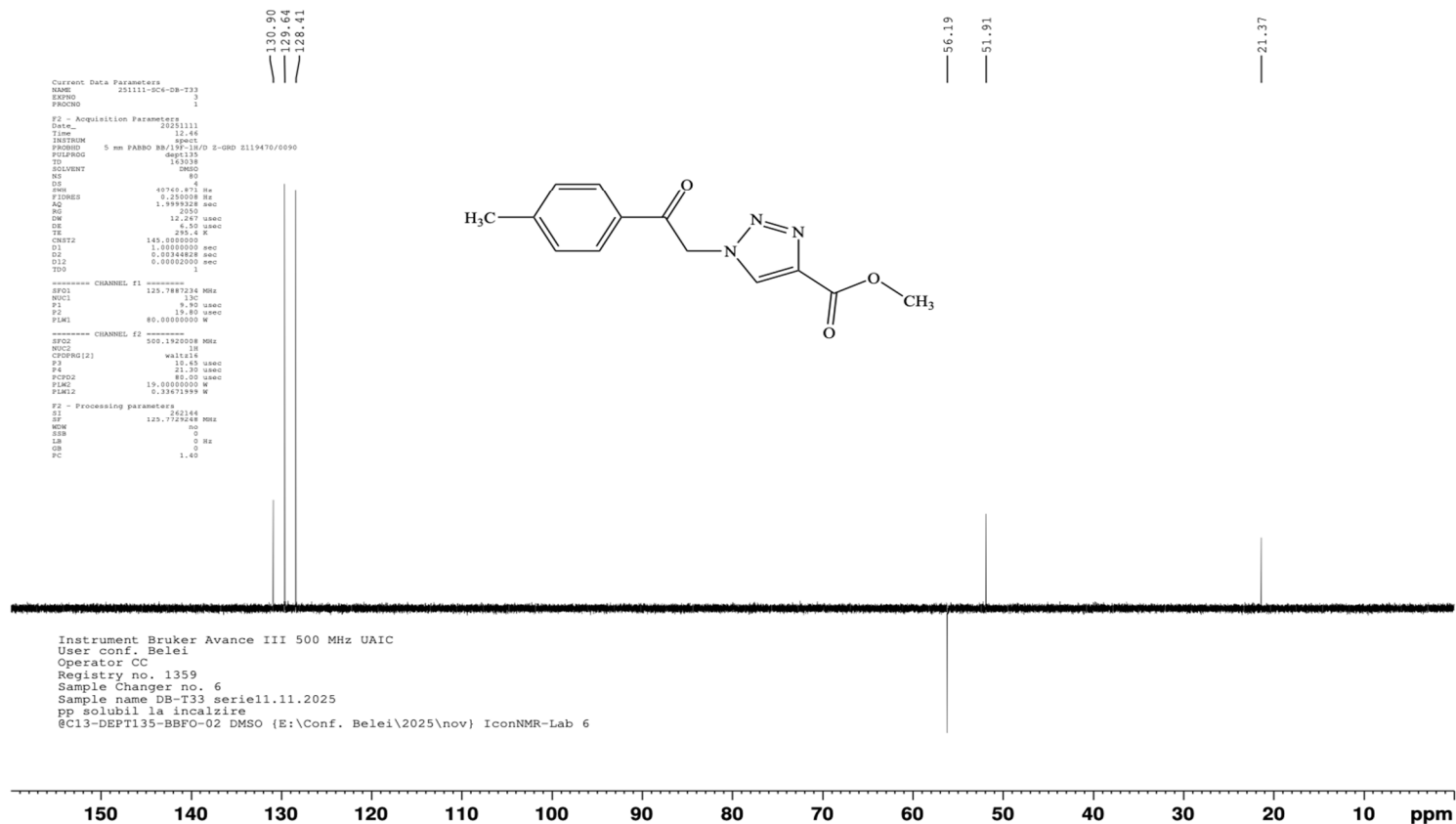


Figure 13. ^{13}C -dept 135 NMR spectrum of **2d** (DMSO- d_6 , 125 MHz).

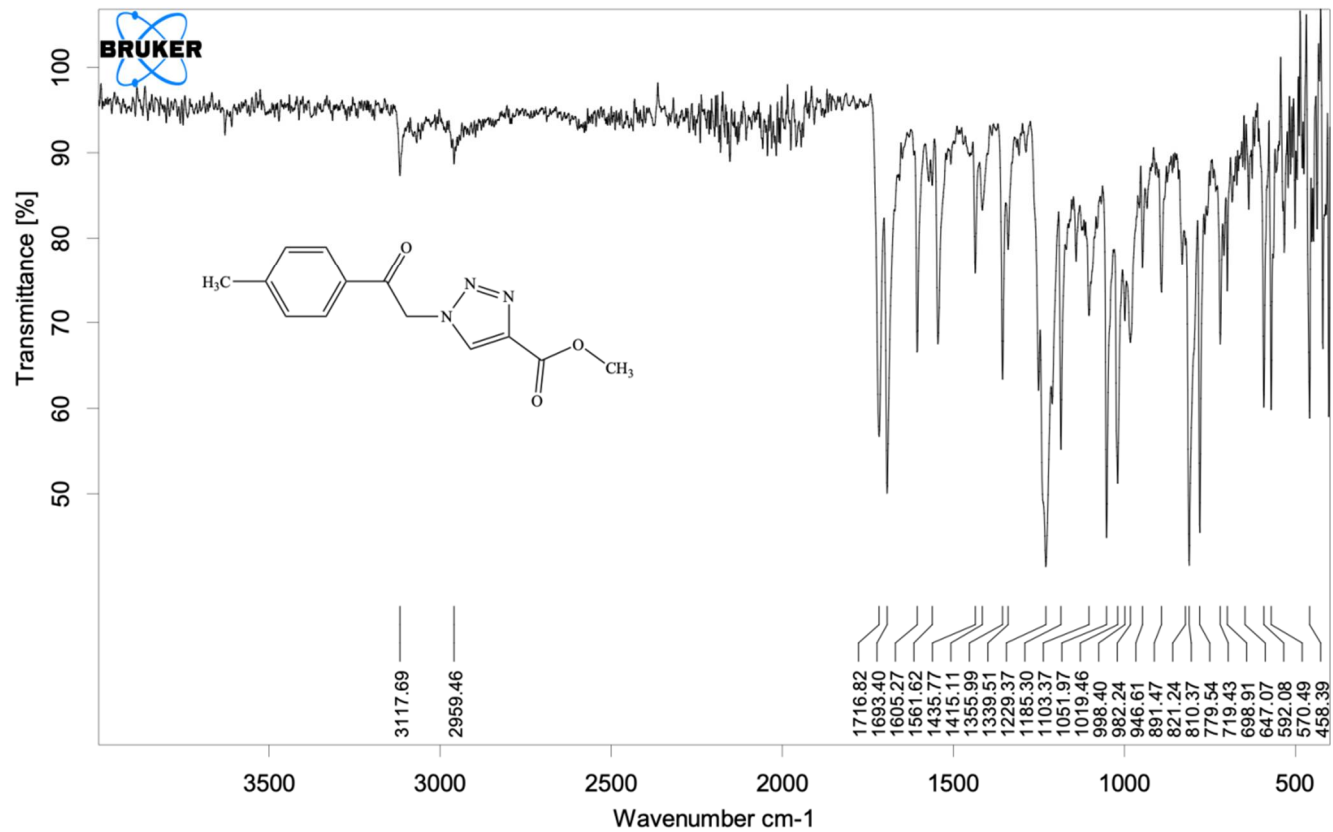


Figure 14. ATR-IR spectrum of **2d**.

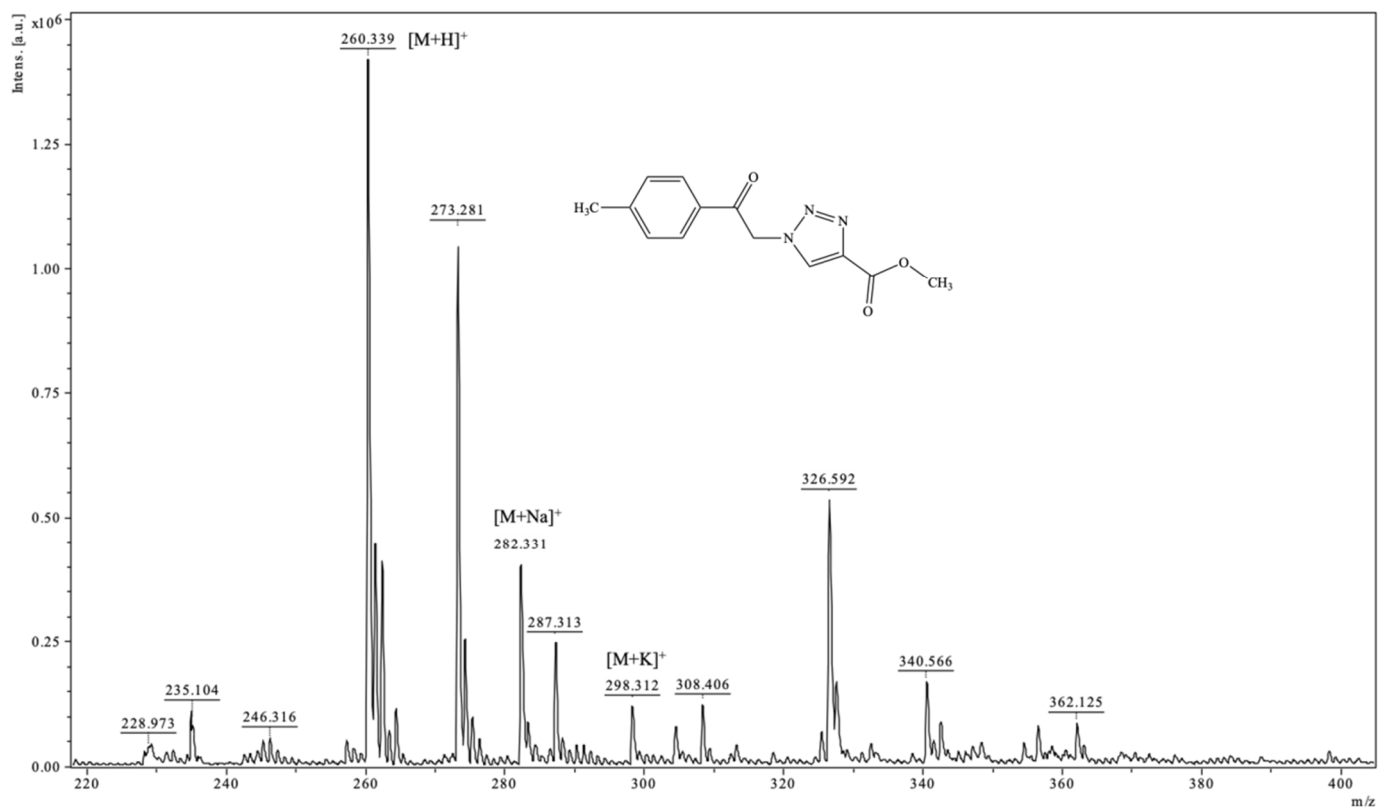
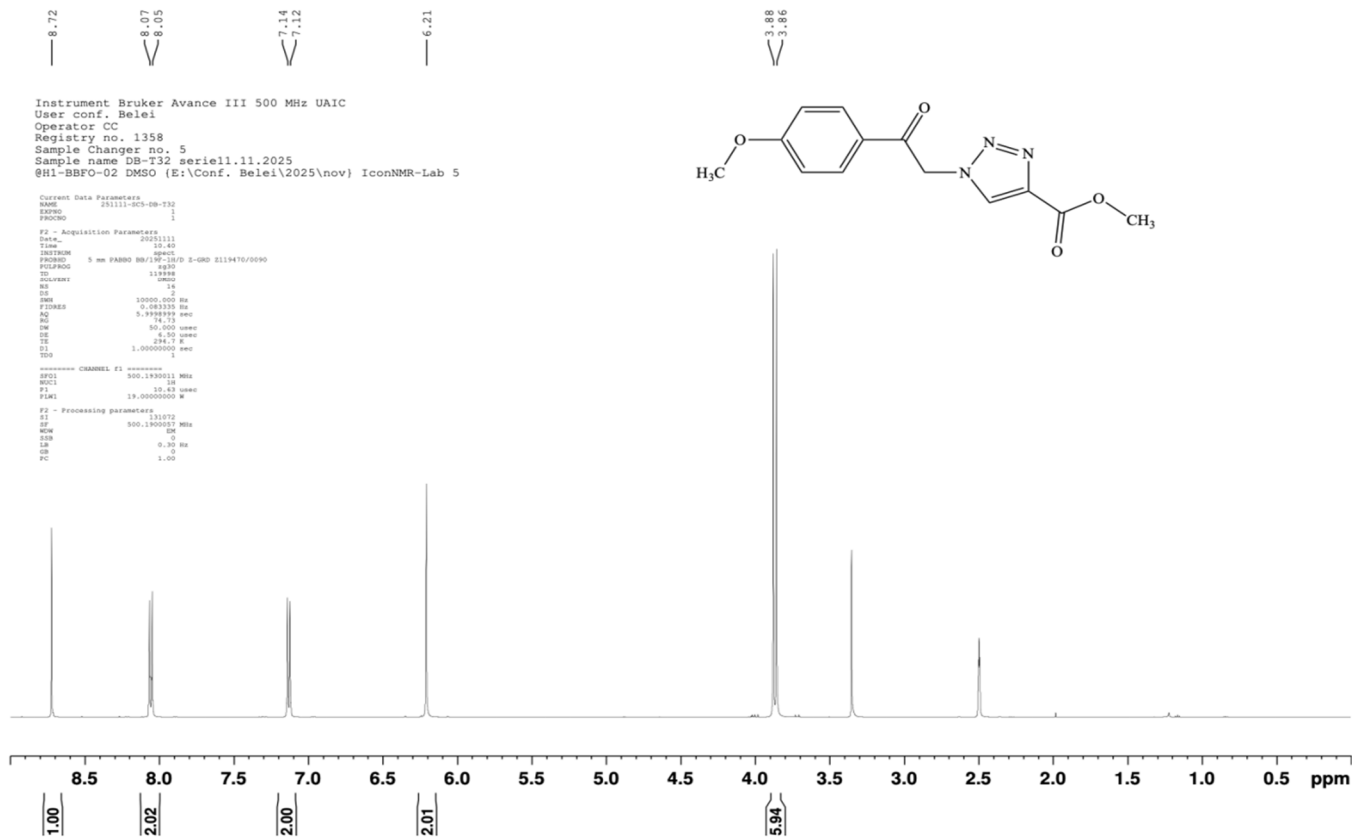


Figure 15. MS spectrum of **2d**.

Methyl 1-(2-(4-methoxyphenyl)-2-oxoethyl)-1H-1,2,3-triazole-4-carboxylate (2e)



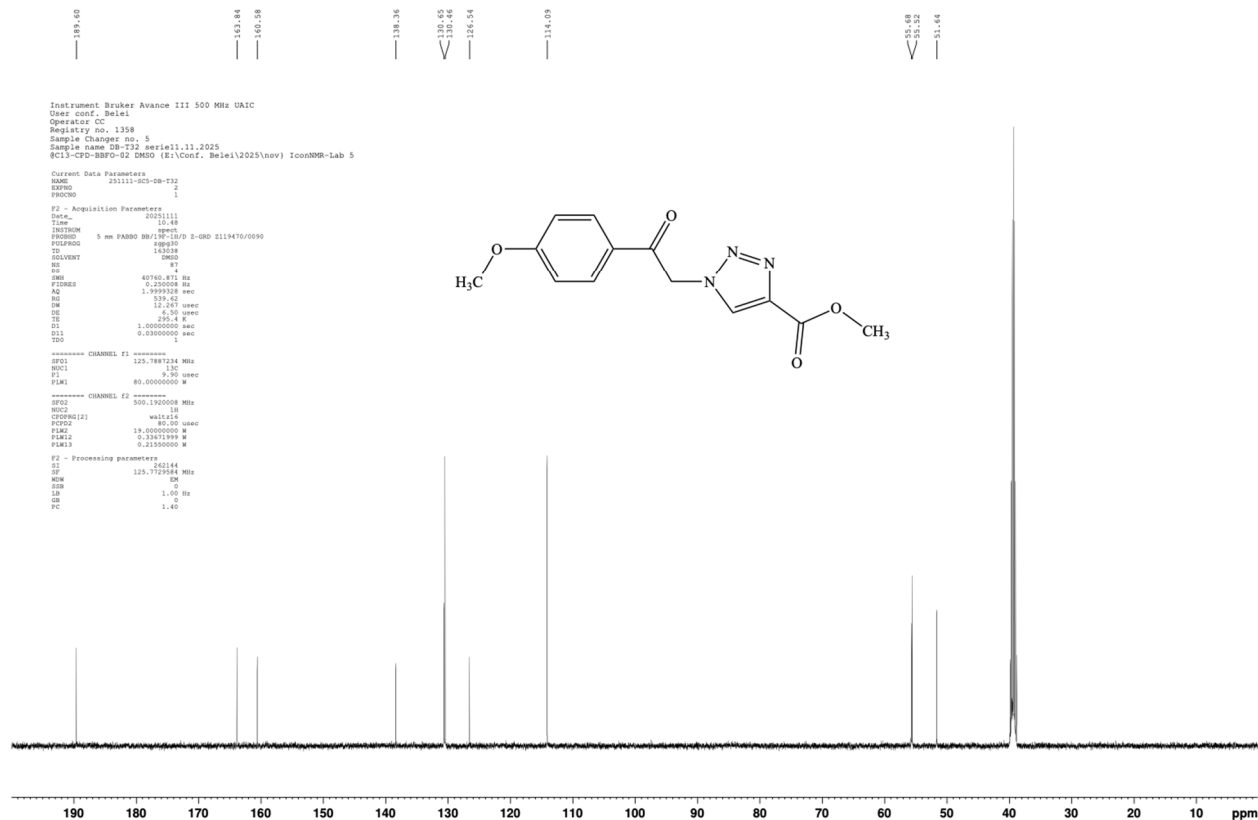


Figure 17. ¹³C NMR spectrum of **2e** (DMSO-*d*₆, 125 MHz).

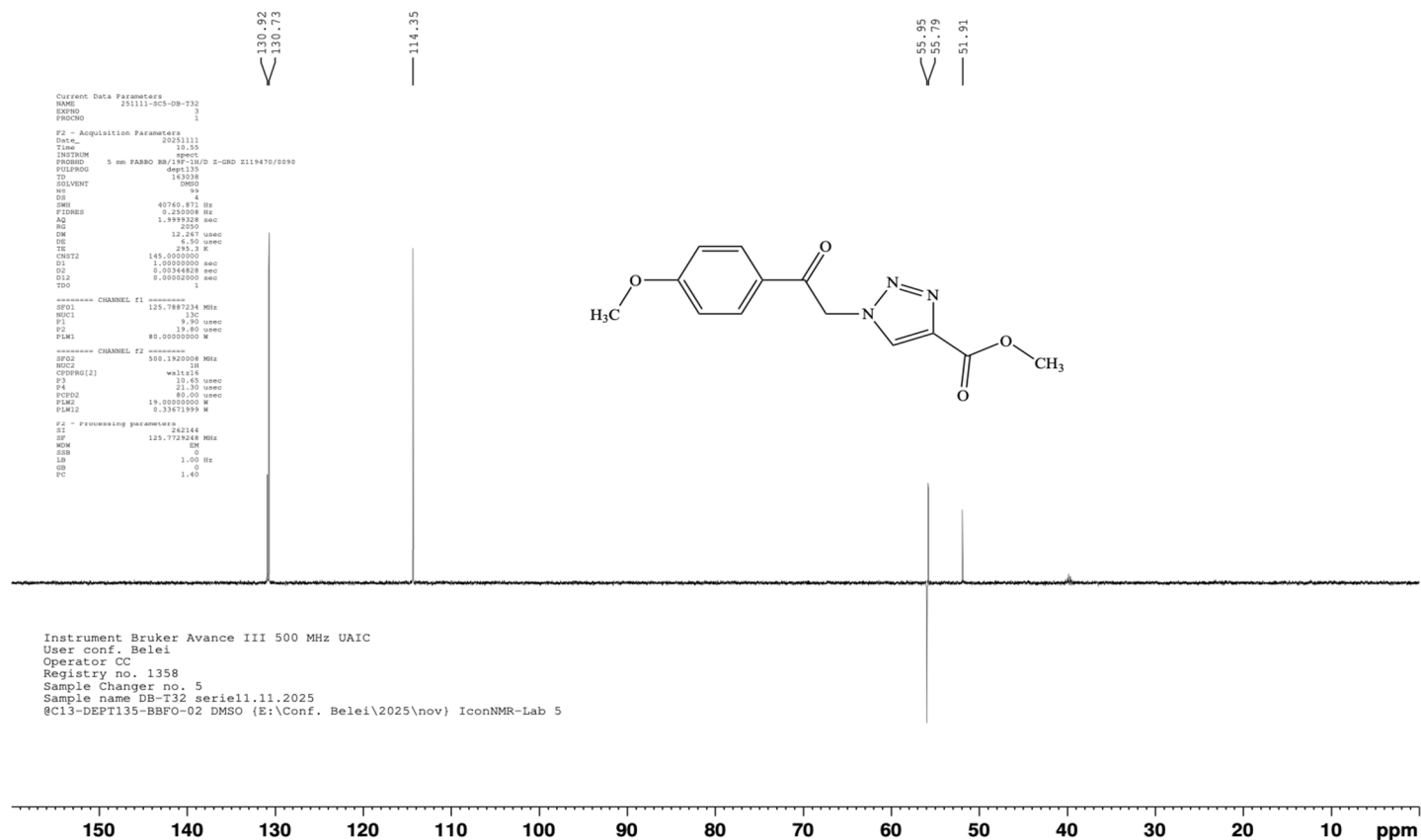


Figure 18. ¹³C-dept 135 NMR spectrum of **2e** (DMSO-*d*₆, 125 MHz).

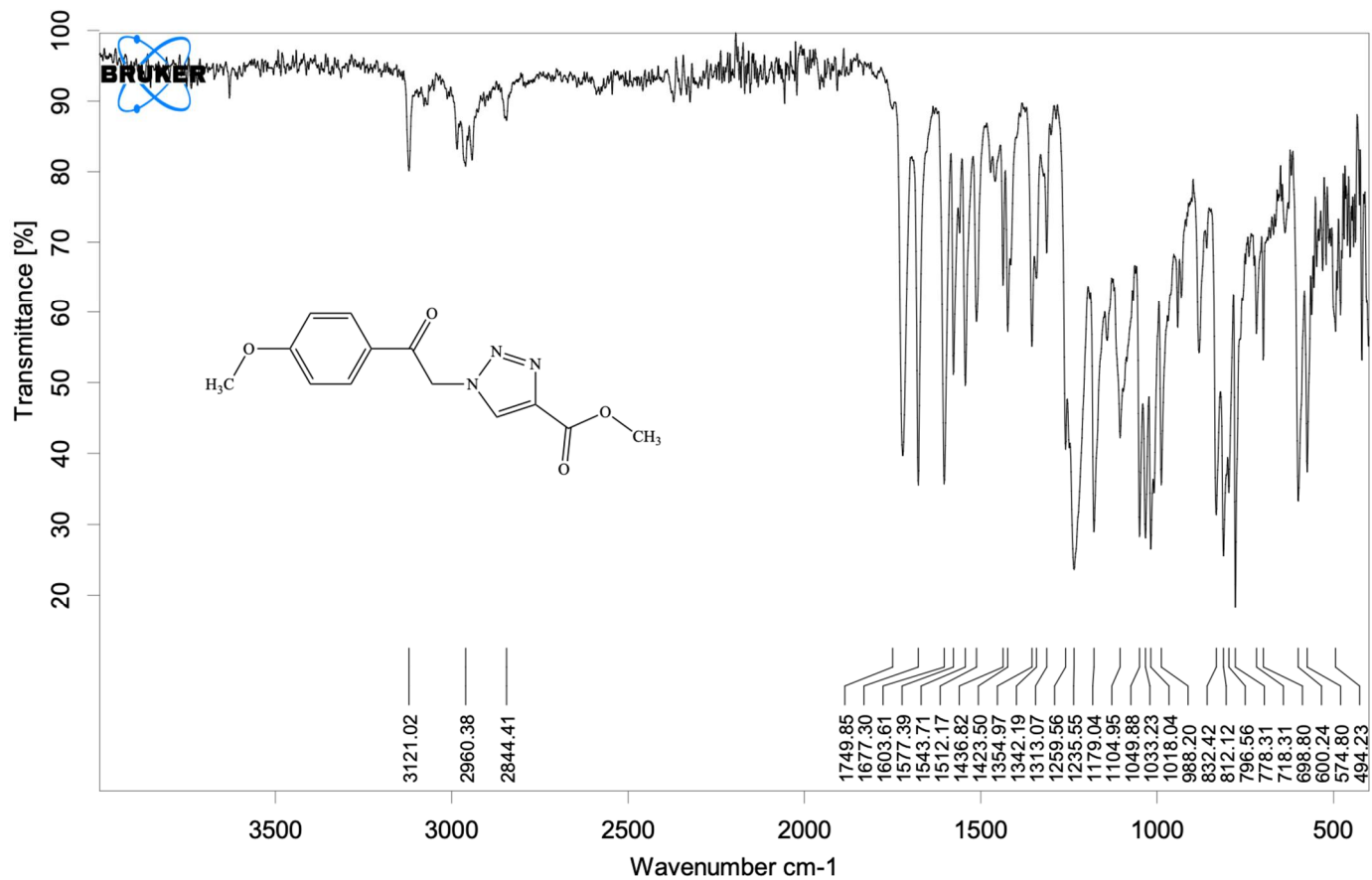


Figure 19. ATR-IR spectrum of **2e**.

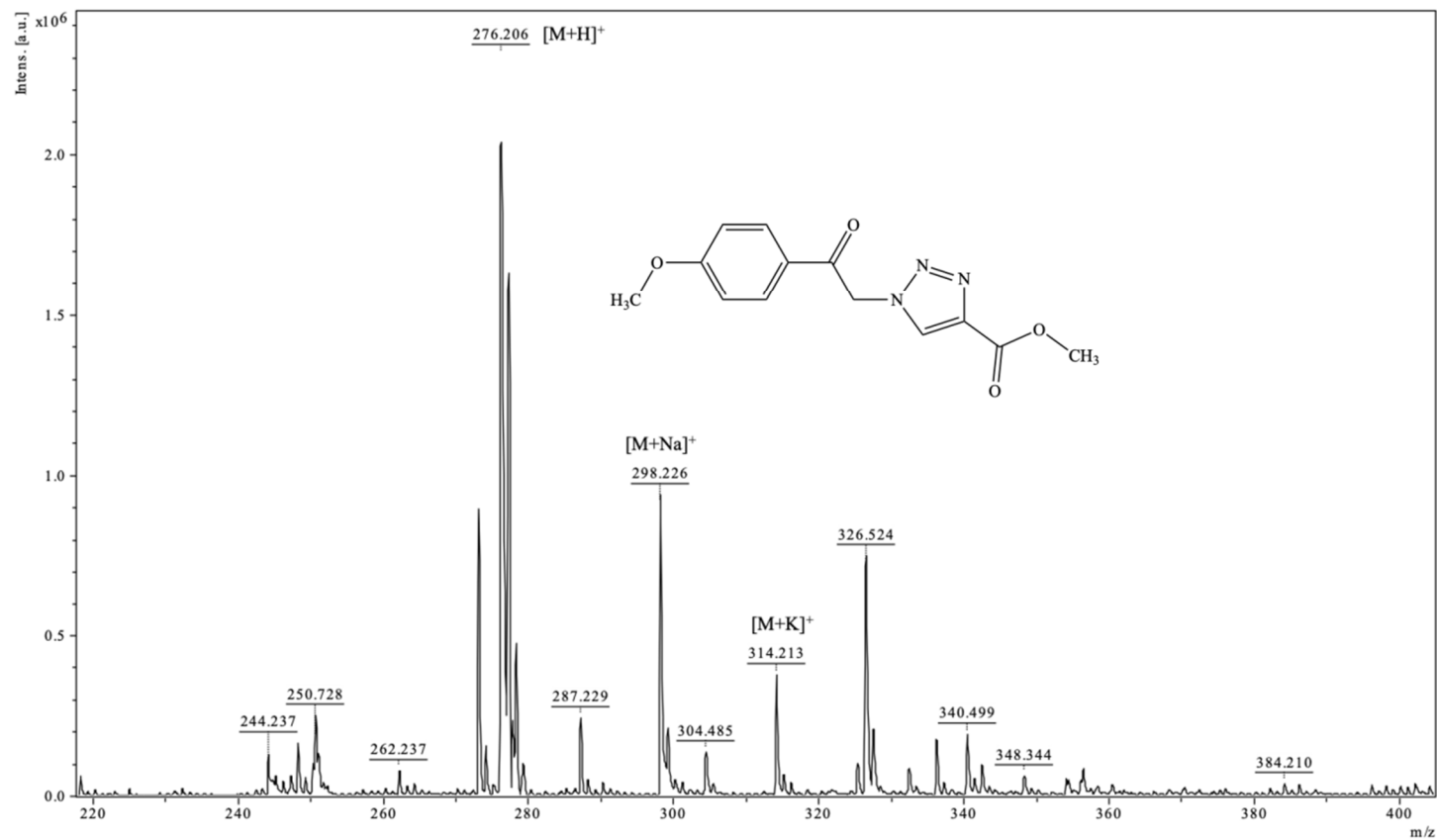


Figure 20. MS spectrum of **2e**.

Methyl 1-(2-(4-chlorophenyl)-2-oxoethyl)-1H-1,2,3-triazole-4-carboxylate (2f)

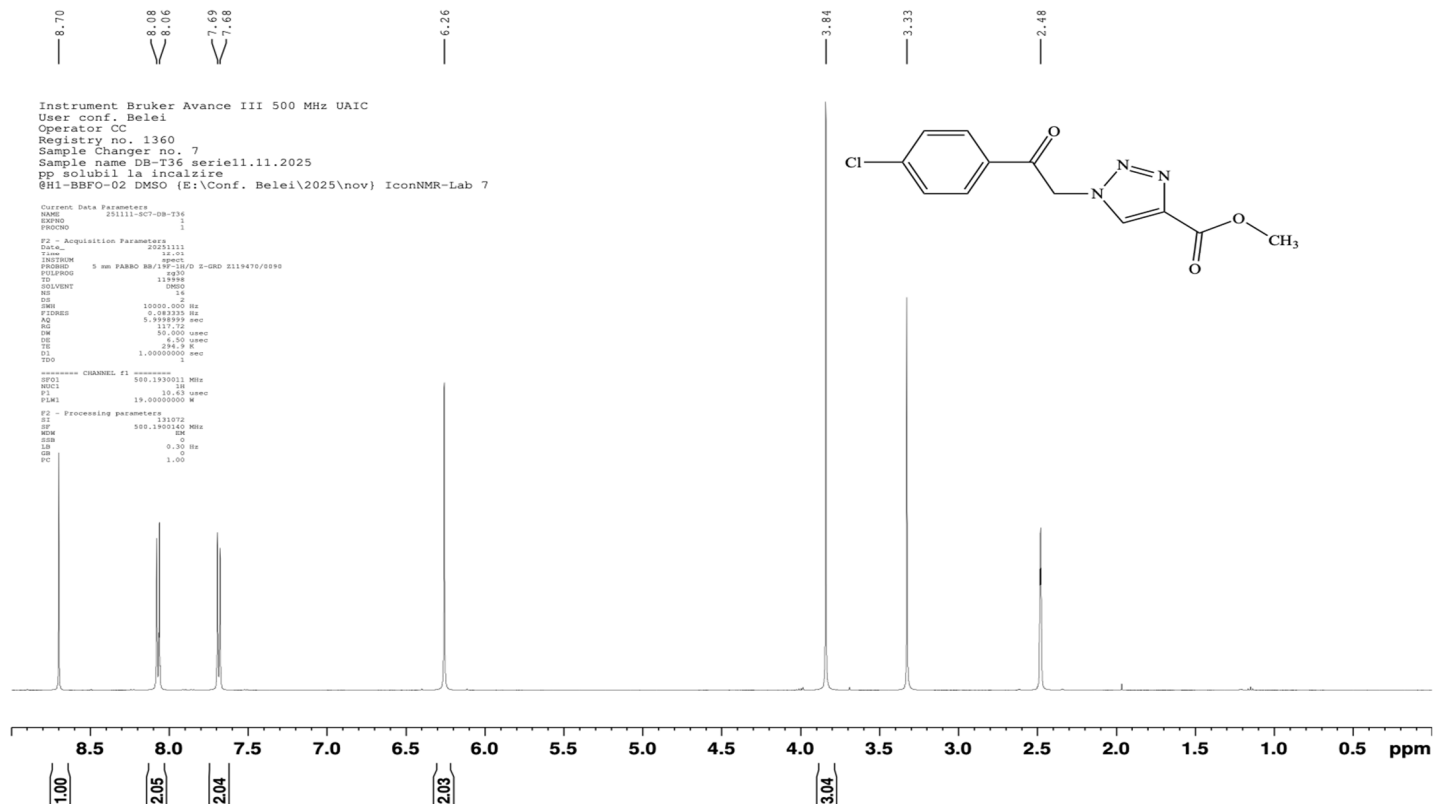


Figure 21. ¹H NMR spectrum of **2f** (DMSO-*d*₆, 500 MHz).

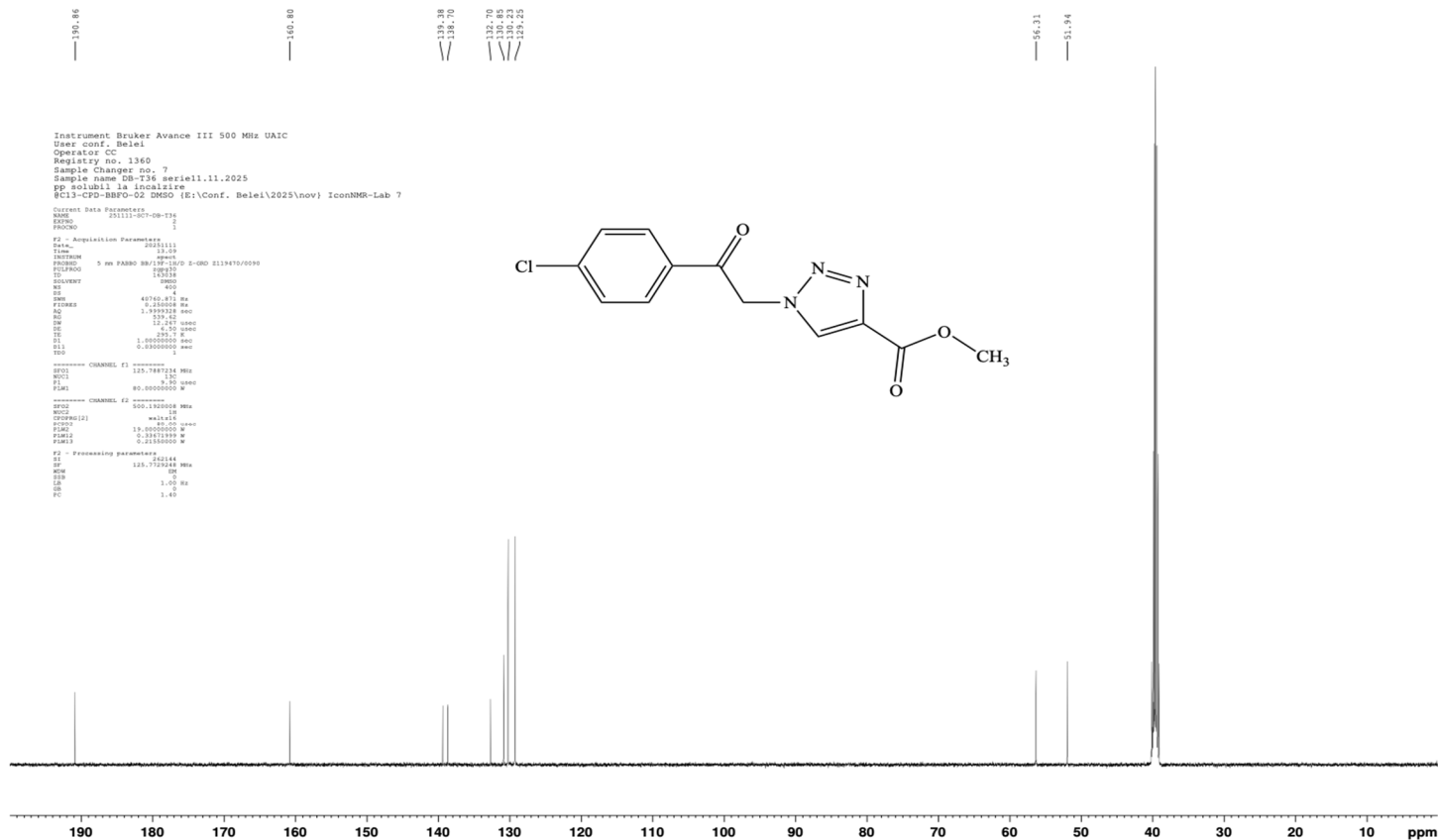


Figure 22. ^{13}C NMR spectrum of **2f** (DMSO- d_6 , 125 MHz).

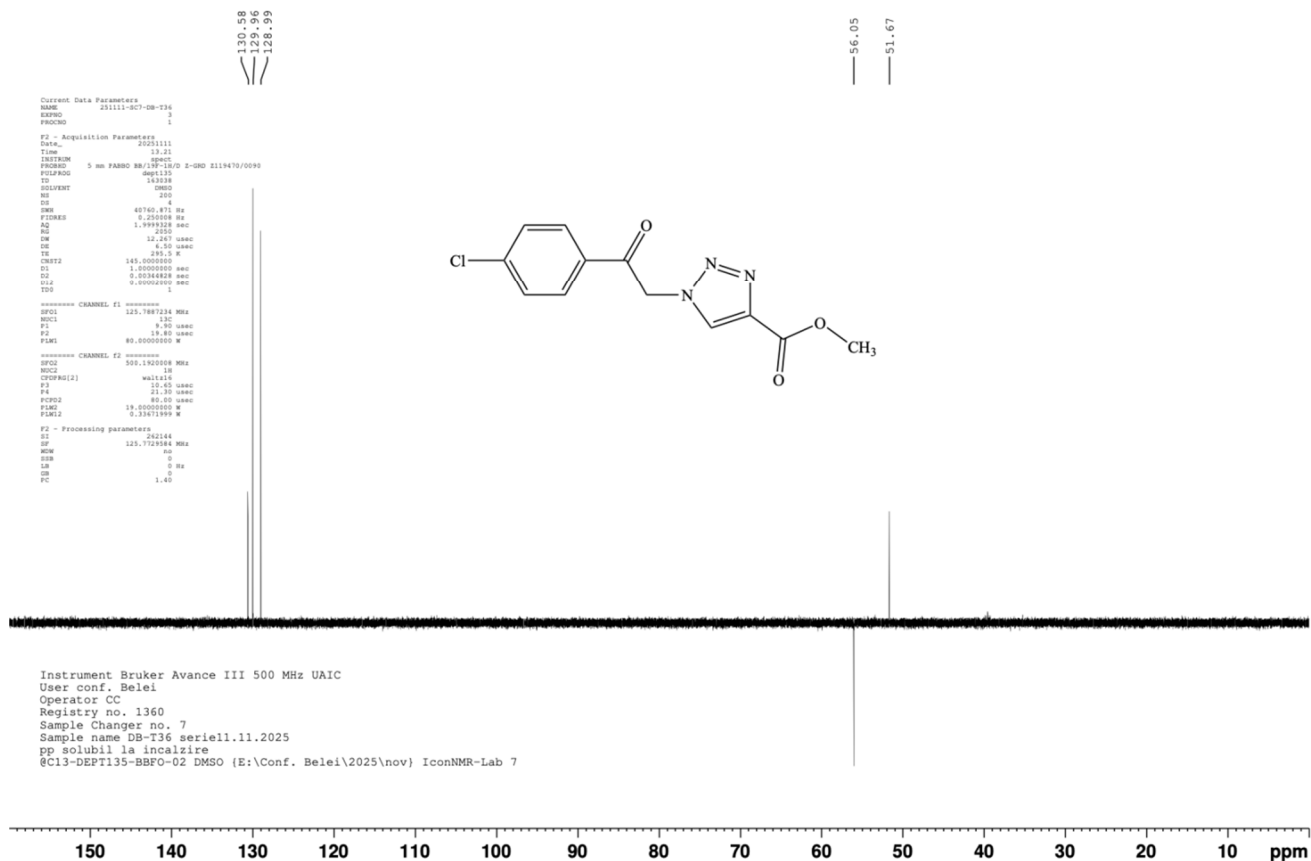


Figure 23. ^{13}C -dept 135 NMR spectrum of **2f** (DMSO- d_6 , 125 MHz).

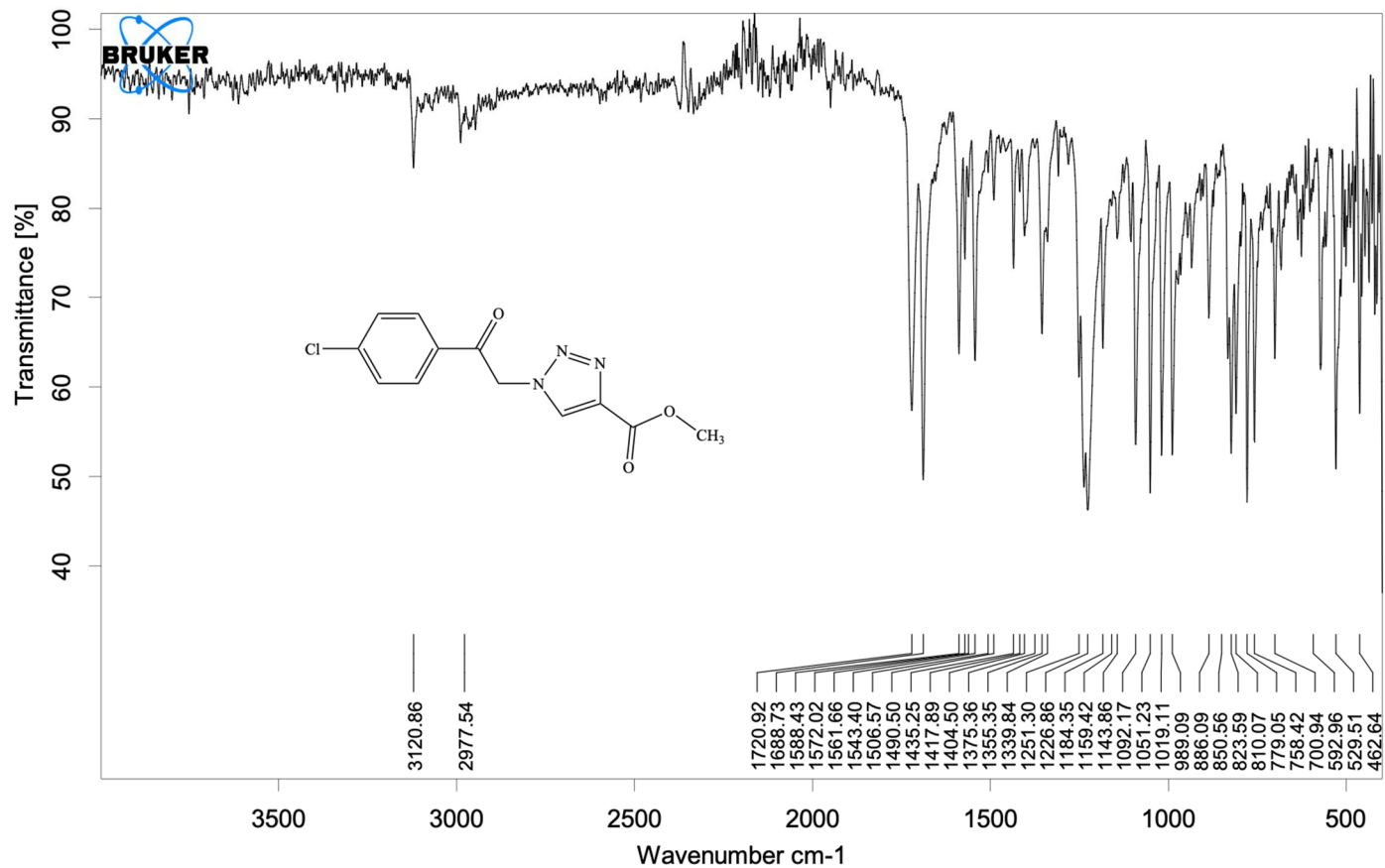


Figure 24. ATR-IR spectrum of **2f**.

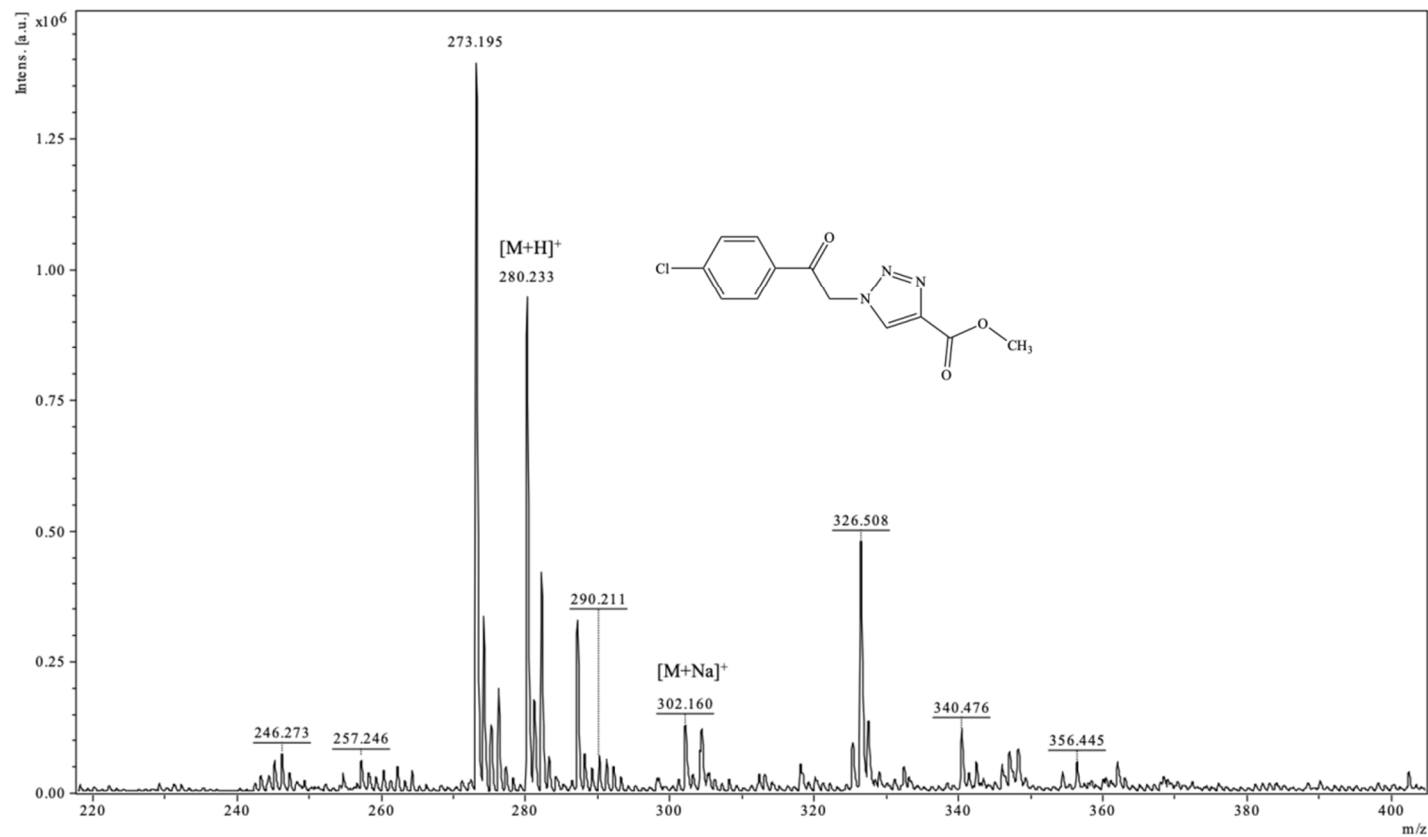


Figure 25. MS spectrum of **2f**.

Methyl 1-(2-(4-cyanophenyl)-2-oxoethyl)-1H-1,2,3-triazole-4-carboxylate (2g)

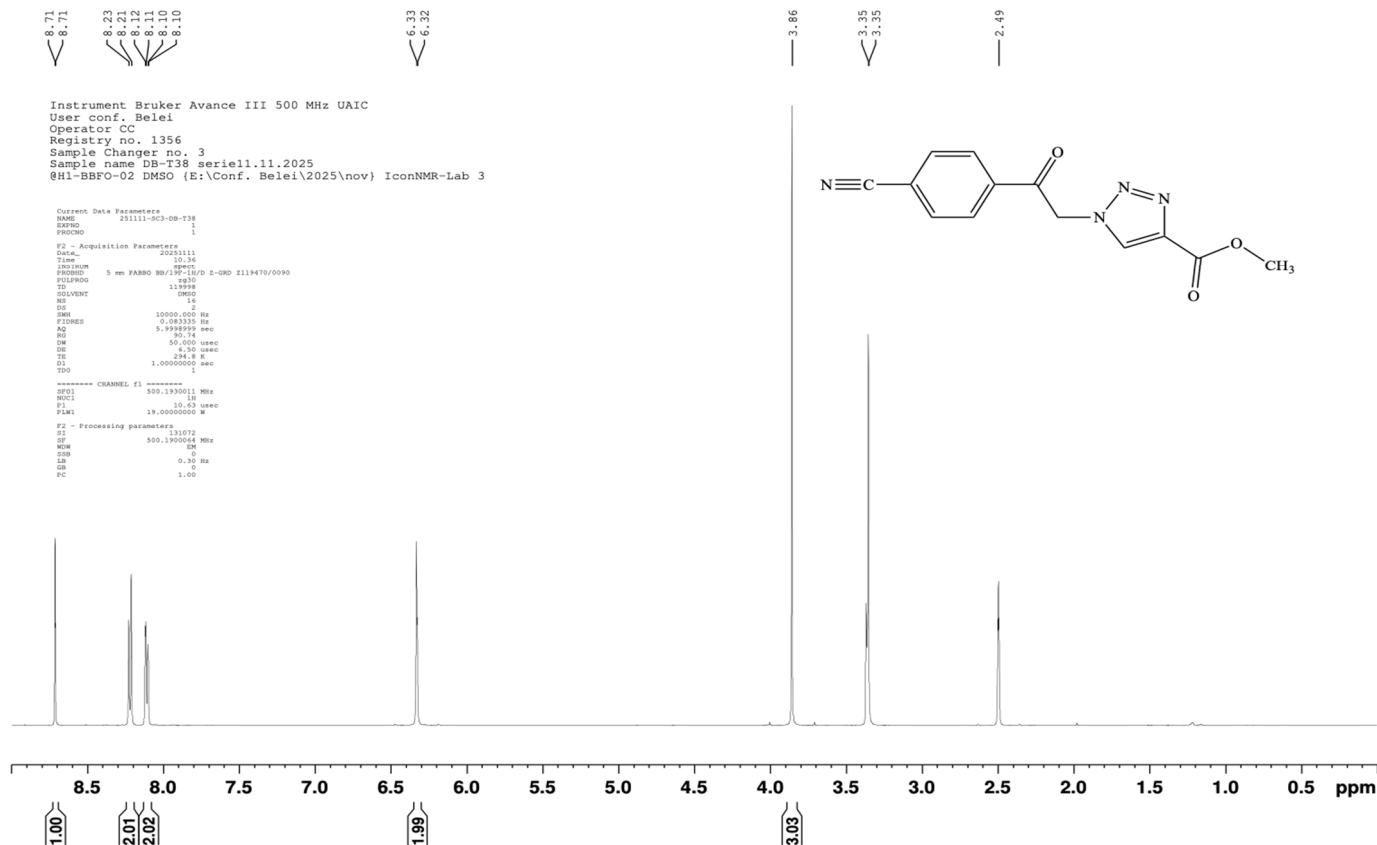


Figure 26. ^1H NMR spectrum of **2g** (DMSO- d_6 , 500 MHz).

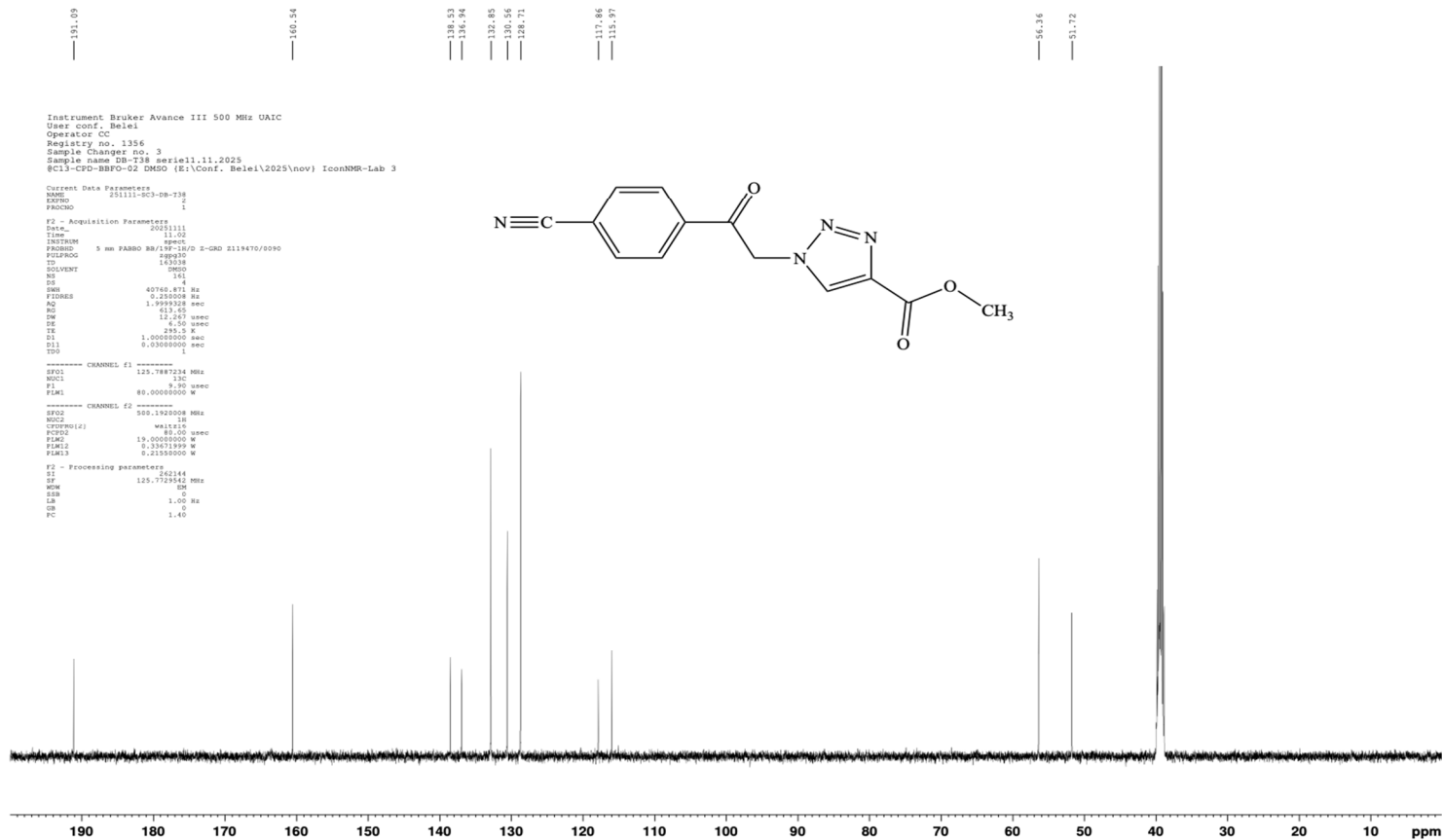


Figure 27. ^{13}C NMR spectrum of **2g** (DMSO- d_6 , 125 MHz).

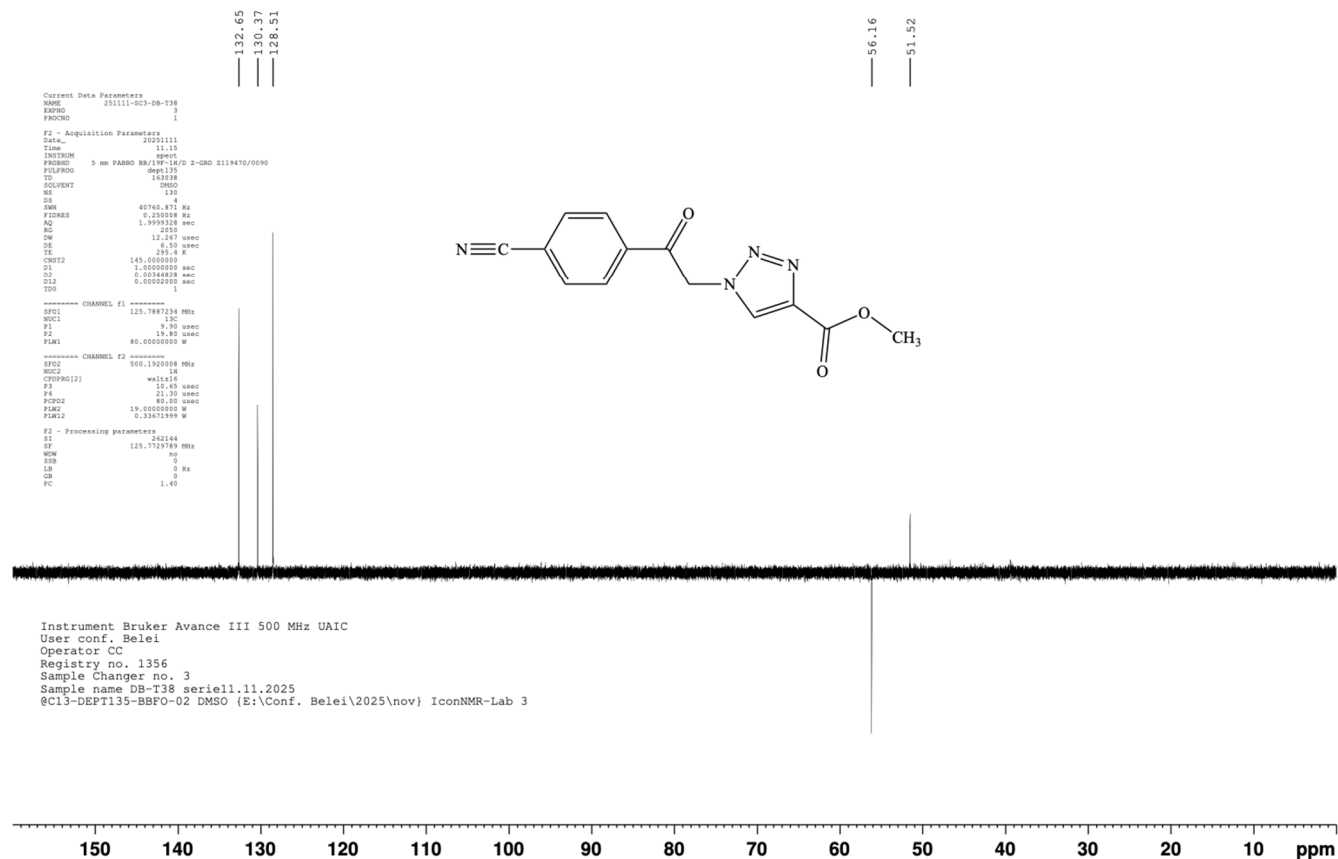


Figure 28. ¹³C-dept 135 NMR spectrum of **2g** (DMSO-*d*₆, 125 MHz).

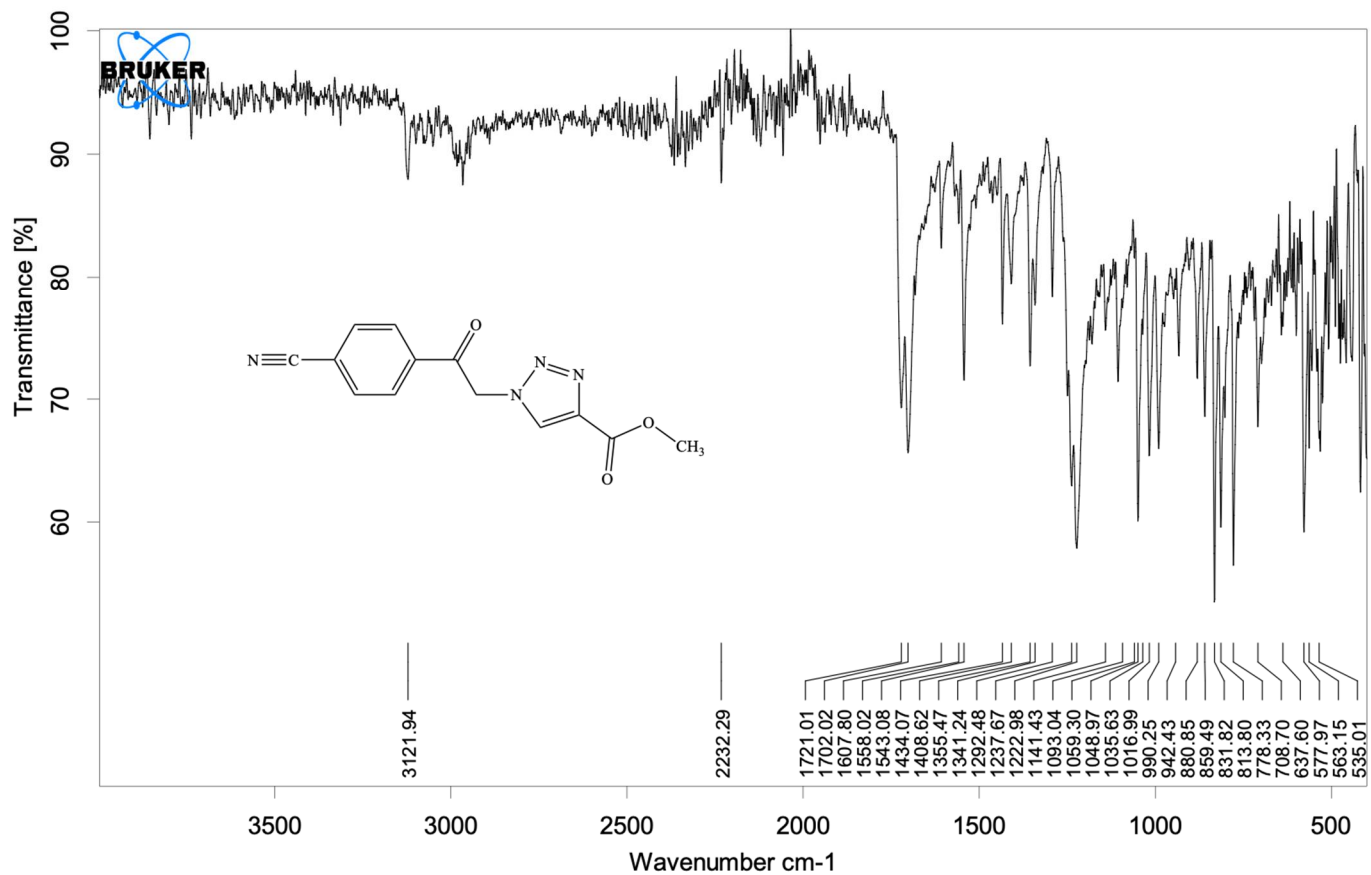


Figure 29. ATR-IR spectrum of 2g.

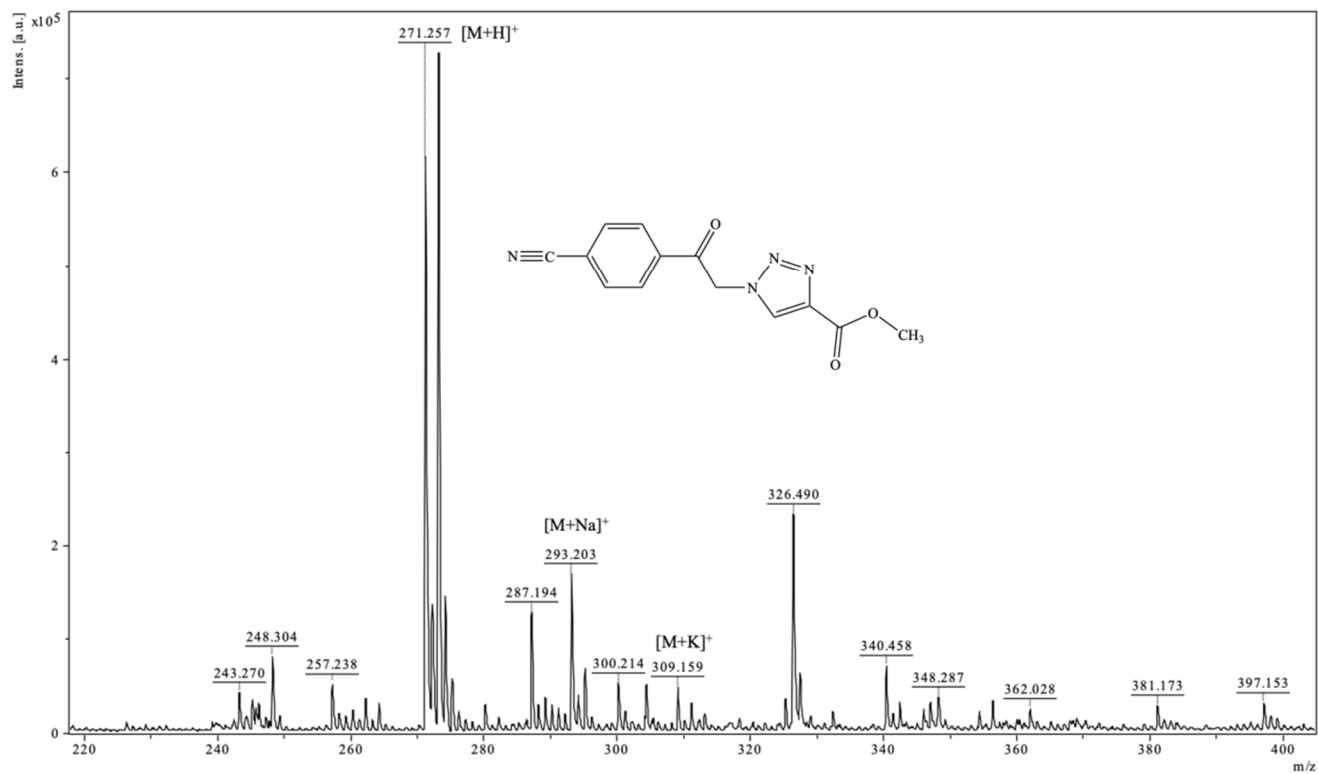


Figure 30. MS spectrum of **2g**.